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Modeling and Theory Support for Mid-IR

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Final Report

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14. ABSTRACT

This report summarizes the technical activity provided under task order 3 of the SLIDERS contract. This task provided for computer modeling and theoretical analysis of mid-IR semiconductor laser materials and device designs. The objective of the effort was to increase the power, brightness and operating temperature of mid-IR semiconductor lasers and laser arrays.

15. SUBJECT TERMS

Energy band modeling, InAs/GaSb superlattices, empirical pseudopotential modeling

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I. INTRODUCTION

The SLIDERS contract encompassed several research efforts within the Semiconductor Laser Branch of the Laser Division, Directed Energy Directorate of the Air Force Research Laboratory. The scope of this contract included development, design, fabrication, procurement, management, operations and maintenance of optical, electronic, and mechanical systems, subsystems, and components. Principal efforts included theory and concept development, design analysis, laboratory operations, and semiconductor laser and diode-pumped laser development, operation and maintenance. Efforts also included the development, procurement, and operation of instrumentation to evaluate and characterize laser systems.

The objective of task order 3 was to provide modeling and theoretical analysis with the objective of increasing the power, brightness and operating temperature of mid–IR semiconductor lasers and laser arrays.

II. MODELING AND THEORY SUPPORT FOR MID-IR SEMICONDUCTOR DEVELOPMENT

Modeling and analysis of mid-IR semiconductor lasers was supported through the development and refinement of an empirical pseudopotential method, applied to thin superlattice structures common in mid-IR laser development work. Work on this method progressed in a number of areas.

We completed a pseudopotential bulk model and began generating the 3-dimensional energy bands and matrix elements for the $InAs_{.90}$ $Sb_{.10}$ ternary. We began work on a 3-dimensional bulk Gain/Index model for narrow band gap semiconductor materials. This code will be used in conjunction with the EPM bulk band model. We also began work on a 3-dimensional bulk Gain/Index code using the effective mass approximation to be used as a quick approximate check on the EPM gain/index model. This model was also used to determine the bulk antiguiding number for 4*u*m material being studied in the lab. The preliminary comparisons to experimental data look very good.

We completed a 4^{th} order polynomial fit to our strained InAs pseudopotential coefficients. These fits were used to determine coefficients for unstrained (Bulk) InAs.

We began work on a new line-shape function for our EPM based gain/index models. The current Lorentzian response function has tails that are too wide and produce a slight absorption below the band edge. This problem is difficult since any new line-shape function must have a phase shift compatible with causality.

We developed both Lorentzian and Tri-linear 3D interpolator algorithms for our bulk gain model. The Lorentzian model proved not as accurate as the Tri-linear model and was abandoned. We upgraded the EPM model to include the ability to run asymmetric edge functions. Using this model we studied InAs/GaAs/GaSb interface designs.

We extended our EPM modeling capability to include both 6 and 12 layer superlattice designs. This upgrade was used to investigate current laser designs.

We began developing a quantum dot version of the EPM Model.

We completed a study of our strain approximation formulation in the EPM code. We feel that our theory gives good results for compressive strain but tensile strain is more approximate. To support this effort we constructed a new bulk EPM code that calculates strain properties exactly. We began working on a functional form for the pseudopotential form factors used in our EPM model. This functional fit will allow us to readily accommodate high levels of hydrostatic &

shear strain. We finished developing the strain code and began using it to look at oscillator strengths between conduction and light & heavy-hole bands

We derived and incorporated into our EPM model, a self consistent band bending algorithm, that looks at some of the many-body affects we previously had neglected.

We are also improving our entire pseudopotential fitting procedure. We're currently using a potential form derived by Kittel. This form allows us to independently adjust the strengths of both the Yukawa like term as well as the constant core term. We are having very good success fitting the gaps, spin-orbit-split offs and conduction & light hole masses. The parameter dependencies of this potential are still being investigated.

We implemented a new potential form into our EPM potential coefficient-fitting model. This form more closely mimics the Yukawa potential as we move away from the atoms core. In addition we developed a new model, which assumes a shielded Yukawa with a repulsive core for the potential form. This model will be used to guide us in determining better fits for the bulk constituents used in our EPM modeling of the MID-IR material systems.

Using our EPM method, we evaluated the AlAs/GaAs superlattice structure using our EPM model. As we thin up the GaAs layer to less than 20 A the electrons confinement switches from the GaAs layer to the AlAs layer. This switch happens because the small GaAs width causes the electron energy to lie above the weakly confined conduction band minimum in the AlAs layer. The AlAs is an indirect material, its conduction band minimum lies at the x-point in the Brillouin zone. These results are in very good agreement with published transitions points for this material system.

We completed work on evaluating barrier thickness' variations in MIT's 6 layer Internal Absorption Quantum Well (IA-QW) lasers.

We investigated why other researchers using the EPM theory have found consistently higher energy levels than observed experimentally. It appears that interface regions are providing artificially high barriers between the different constituent materials thus in effect isolating each of the well regions in the superlattice structure.

We completed fits for the 8ML/24ML luminescence vs pump experimental data to the luminescence -vs- sheet carrier density theoretical results calculated from the EPM model. These led to pump - vs - carrier density curves, which were fit with the standard $AN + BN^2 + CN^3$ carrier recombination law. From these fits we can determine Shockley-Reed, Radiative Recombination and Auger parameters

We completed the modeling of the full dispersion band energy curves for two W-laser structures. The two devices differ in the amount of Indium in the Ternary layer (20% & 30%). The band dispersions were used to help us ascertain the T_0 characteristics of each device. We completed Gain -vs- Temp (constant inversion) and Inversion -vs- Temp (constant Gain) studies for each device

We completed empirical pseudopotential model (EPM) calculations for 20%, 25%, 30% & 35% Indium concentration levels for W-lasers. We used these calculations to examine the V1-V2 (valence band) separations versus varying strain levels.

We began looking at material offsets (Quat-Tern & Ternary-InAs) and how these affect our EPM predicted device break points on recently developed type-II optically pumped semiconductor lasers.

We designed a low divergence 'outrigger' waveguide. This design was incorporated into the 4 μm W-laser active region. The laser device was processed and we are currently waiting on test results to see if the waveguide will achieve the low lateral divergence predicted from our models.

We used our EPM modeling capabilities to verify the digital alloy approach to growing the quaternary material, (InGaSbAs). Our results indicated that for thin enough binary (InAs/GaSb) layer combinations, the digital alloy method of forming the quaternary works well.

We found EPM coefficients for two new ternary materials (InGaSb) (15% & 25%) for use in our superlattice EPM model. These new fits were used to investigate the effects of increasing indium concentrations in the ternary section of the four component W-laser structure (Quat/InAs/Tern/InAs). Our modeling efforts indicated that increasing the percentage of indium increased the devices performance characteristics (T0, T1). This was in excellent agreement with observed experimental data taken from devices grown by members of Directed Energy Laser Systems.

We derived and verified an offset rule between InAs & InGaSb that varies with indium concentration in the ternary. It was previously thought that this offset was a constant.

We completed the *sbend* model to accurately determine the effects of band bending in type-II superlattice structures. We completed a series of runs on the QB (Quaternary/InAs) superlattice active region, the results are in excellent agreement with experimental measurements.

In addition to the EPM model, we completed a steady-state thermal model to enable us to analyze the power extraction from an optically pumped semiconductor laser as a function of heat sink temp. We also completed and debugged a full, time-dependent power extraction model for optically pumped semiconductor lasers (OPSL's). We sent preliminary results on active region temperature increases for 50, 5, and 2.5 microsecond pulse widths, for 200 μm and 100 μm stripe widths, to MIT. This temperature model includes full (x, z, time) dependence.

In other efforts, we provided an analytic expression for the exchange length between the coupled modes in an alpha-DFB laser structure using a degenerate mode approach. This expression and some numerical modeling support was provided to Dr. Gary Evans of SMU in conjunction with his 1.55um alpha-DFB laser design project.

We completed an analysis of the effects of low confinement (fill) factor on the filament formation process in broad area semiconductor lasers. We are currently preparing an open literature article of these results.

We completed dielectric waveguide calculations for alpha-DFB waveguide devices from MIT and Sarnoff. The reflection operator method appears to working well for pure dielectric waveguide cases while the results for cases with complex index of refraction are suspect.

We worked on a model for spontaneous emission and amplified vacuum field effects in an etalon. This will be used for improved analysis of the Hakki-Paoli experiments currently being performed in the lab. We found that both reflective and transmissive regenerative gains must be included to accurately fit FTIR sub-threshold spectral data.

Also in support of the Hakki-Paoli experiments, we completed an analysis to convolve the FTIR instrument function with the etalon response function that is currently being used in the gain/index measurements. We developed a Fourier series representations for various instrument functions (Lorentzian, Sinc & Sinc**2).

III. PUBLICATIONS AND PRESENTATIONS

Publications

"*Optically Pumped Integrated Absorber 3.4 μm Laser With InAs-to-InGaAsSb Type-II Transition*"**,** Applied Physics Letters, in press.

"*As-soak Control of the InAs-on-GaSb Interface*", J. Crystal Growth, 225, (2001) 544

"*Spectral blueshift and improved luminescent properties with increasing GaSb layer thickness in InAs-GaSb type-II Superlattices*", J. Appl. Phys. 89, (2001) 2185

"*Response Surface Modeling of the Composition of $AlAs_ySb_{1-y}$ Alloys Grown by Molecular Beam Epitaxy*" , J. Crystal Growth, 225, (2001)556

"*Visualizing interfacial structure at non-common-atom heterojunctions with cross-sectional STM*", Phys. Rev. Lett. 85, (2000) 2953

"*Improved procedure for determining gain, differential index and α-parameter using below-threshold spectra of mid-IR semiconductor lasers*", submitted to Applied Physics Letters

"*Low confinement factors for suppressed filament formation in semiconductor lasers*", submitted to Applied Physics Letters

"*High-power optically-pumped type-II lasers with integrated absorber layers*", submitted to the Journal of Applied Physics

Presentations

"Spectral Blue Shift and Improved Luminescence Properties with Increasing GaSb Layer Thickness in InAs/GaSb Type-II Superlattices", 42nd Electronic Materials Conference, Denver CO.

"Optically-pumped type-II lasers with integrated absorber layers", International Conference on Mid-IR Optoelectronics Materials and Devices, April 2001

"Empirical pseudopotential methods for type-II band-structure calculations", 31st Winter Colloquium on The Physics of Quantum Electronics, Salt Lake City, UT, January 2001.

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